

# Operator equation of motion in phase space and path integral solution to time-dependent systems possessing invariants : Application to time-dependent harmonic oscillator

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**Abstract** : The phase space distribution function provides a basis for discussing quantum phenomena within a classical-like framework. The equation of motion for the Wigner operator in phase space derived earlier (S K Ghosh and A K Dhara *Phys. Rev. A* **44** 65 (1991)) is employed here to propose a new approach for obtaining a path integral solution to the phase space distribution function for time-dependent systems possessing invariants. For a time-dependent harmonic oscillator, the solution for the phase space distribution function is obtained by mapping the corresponding results for a free particle using suitable variable transformations. The viability of the phase space route and applicability of the proposed method to the investigation of general time-dependent properties of molecular systems is discussed.

**Keywords** : Phase space distribution function, operator equation of motion, phase space propagator, path integral solution

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## 1. Introduction

The phase space (PS) formulation of quantum mechanics [1–4] provides a framework to discuss quantum phenomena in terms of a classical-like distribution function in phase space and thereby calculate quantum mechanical expectation values using simple integration, with position and momentum being treated as ordinary variables rather than as operators. Although the Wigner PS function is defined through a partial Fourier transform involving the wavefunction in coordinate or momentum space, its calculation through this route is difficult even for very simple systems. The equation governing the time-evolution of the PS function has, therefore, directly been employed

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in a wide variety of applications [4] such as collision phenomena, intramolecular energy transfer, photodissociation *etc.*

The quantum mechanical PS formalisms have mostly been discussed in terms of the distribution functions. The equations determining these functions, however, involve phase space operators, known as Wigner operators (essentially Bopp operators [3]), which although are not needed for evaluating the expectation values, play an important role in the PS formulation of quantum mechanics. Although the equations governing the PS function have been studied extensively, the equation of motion for the Wigner operators, which represent the PS analogue of the Heisenberg equation of motion for a quantum mechanical operator, have been derived rather recently [5].

The quantum Liouville equation governing the time-evolution of the PS function is, however, not a simple differential equation but involves series expansion in the derivatives with respect to both position and momentum coordinates and hence cannot be solved very easily. It is therefore highly important to develop methods for solving these equations. In this work, we obtain a path integral solution for the PS distribution function, using the operator equation of motion derived [5] by us earlier, for a certain class of time-dependent (TD) problems, *viz.* those associated with TD invariants [6], which includes problems involving a TD harmonic oscillator or a charged particle moving in a TD magnetic field.

The plan of the paper is as follows. In Section 2, we present a brief review of Wigner distribution function and the new phase space operator equation of motion [5]. The path integral solution for the PS function through the operator equation is then obtained in Section 3 for general TD systems possessing invariants and the TD harmonic oscillator as a special case. Finally we offer a few concluding remarks in Section 4.

## 2. Wigner distribution function and the operator equation in phase space

The Wigner distribution function  $f(q, p)$  is defined in terms of the off-diagonal elements of the density matrix through a partial Fourier transform given by

$$f(q, p) = (2\pi\hbar)^{-1} \int dy \exp[ipy/\hbar] \langle q - y/2 | \hat{\rho} | q + y/2 \rangle, \quad (1)$$

and satisfies the properties

$$\int dq f(q, p) = \langle p | \hat{\rho} | p \rangle; \int dp f(q, p) = \langle p | \hat{\rho} | q \rangle; \int dq \int dp f(q, p) = 1. \quad (2)$$

While eq. (1) yields the PS function corresponding to the density operator  $\hat{\rho}$ , its generalization given [2,3,7] by the Wigner-Moyal transform

$$A_s(p, q) = \int dy \exp[ipy/\hbar] \langle q - y/2 | \hat{A} | q + y/2 \rangle, \quad (3)$$

yields the Wigner equivalent PS function  $A_s(q, p)$  corresponding to any quantum

mechanical (QM) operator  $\hat{A}(q, \hat{p})$  with  $\hat{p} = -i\hbar(\partial/\partial q)$ . Eq. (3) essentially represents the reverse process of the Weyl transform for obtaining a QM operator equivalent of a classical PS function. The PS functions corresponding to eqs. (1) and (3) yield the expectation values through a simple classical-like procedure, viz.

$$\text{Tr}(\hat{\rho}\hat{A}) = \int dq \int dp A_s(q, p) f(q, p). \quad (4)$$

For the PS function  $A_s(q, p)$ , one also defines the corresponding Wigner PS differential operator  $\hat{A}_w(q, p)$  as

$$\hat{A}_w(q, p) = A_s(\hat{Q}, \hat{P}), \quad (5)$$

where  $\hat{Q}$  and  $\hat{P}$  are the Bopp operators [7,8] given by

$$\hat{Q} = q - (\hbar/2i)(\partial/\partial p); \quad \hat{P} = p + (\hbar/2i)(\partial/\partial q). \quad (6)$$

The operator  $\hat{A}_w(q, p)$ , when operates on unity, yield the corresponding PS function  $A_s(q, p)$ .

Using these relations among  $\hat{A}(q, \hat{p})$ ,  $A_s(q, p)$  and  $\hat{A}_w(q, p)$ , the equation of motion for the density operator  $\hat{\rho}$ , viz.

$$i\hbar(\partial\hat{\rho}/\partial t) = [\hat{H}, \hat{\rho}] \quad (7)$$

can easily be transformed [3] into the quantum Liouville equation determining the time evolution of the PS distribution function  $f(q, p, t)$ , given by

$$(\partial f/\partial t) = i\hat{L}f(q, p, t), \quad (8)$$

where  $\hat{L}$  is the quantum Liouville operator defined in terms of the Wigner operator  $\hat{H}_w$  and its complex conjugate  $\hat{H}_w^*$  corresponding to the Hamiltonian  $\hat{H}$ , viz.

$$i\hat{L} \equiv (i\hbar)^{-1} [\hat{H}_w - \hat{H}_w^*]. \quad (9)$$

Expansion of eq. (8) in power series of  $\hbar$  restores the classical Liouville equation in the limit  $\hbar \rightarrow 0$  and also makes the quantum corrections explicit and transparent.

Analogously, the equation of motion for a general quantum mechanical operator  $\hat{A}(q, \hat{p})$ , viz.

$$(d/dt)\hat{A} = (\partial/\partial t)\hat{A} + (i\hbar)^{-1}[\hat{A}, \hat{H}] \quad (10)$$

can also be transformed into the PS equation, given by

$$(d/dt)A_s(q(t), p(t), t) = (\partial/\partial t)A_s(q(t), p(t), t) - i\hat{L}A_s(q(t), p(t), t). \quad (11)$$

While these equations for the PS functions correspond to the Schrödinger picture of QM, we have earlier derived [5] an equation of motion for the Wigner PS operator  $\hat{A}_w$ , viz.

$$(d/dt)\hat{A}_w = (\partial/\partial t)\hat{A}_w - (i\hbar)^{-1}[\hat{H}_w\hat{A}_w - \hat{A}_w\hat{H}_w], \quad (12)$$

which is the PS analogue of the Heisenberg equation of motion for the corresponding quantum mechanical operator  $\hat{A}(q, \hat{p})$  in Hilbert space.

For Hamiltonians with general potentials, eqs. (8) and (11) become, in general, partial differential equations of infinitely high order and hence are not easy to solve. However, for a class of potentials (time-dependent systems possessing invariants), the PS operator equation of motion of eq. (12) provides a new path integral solution for the PS function, which we now discuss in the following Section.

### 3. Path Integral solution for the phase space distribution function for the time-dependent systems possessing invariants

The PS distribution function  $f(q, p, t)$  can be expressed as the integral

$$f(q, p, t) = \iint dq_0 dp_0 K(q, p, t | q_0, p_0, t_0) f(q_0, p_0, t_0), \quad (13)$$

where  $K(q, p, t | q_0, p_0, t_0)$  is the PS propagator and is related to the position space propagator  $K(q, t | q_0, t_0)$  by the simple transform [9]

$$K(q, p, t | q_0, p_0, t_0) = \iint dy dy_0 \exp[(ipy/\hbar) - (ip_0 y_0/\hbar)] \\ K^*(q + y/2, t | q_0 + y_0/2, t_0) K(q - y/2, t | q_0 - y_0/2, t_0). \quad (14)$$

Eq. (13) can be employed for the calculation of  $f(q, p, t)$  once the propagator  $K(q, p, t | q_0, p_0, t_0)$  is evaluated and the initial condition, i.e. the value of  $f(q_0, p_0, t_0)$  (denoting  $f(q_0, p_0, t)$  at  $t = t_0$ ) is known for all values of  $q_0$  and  $p_0$ .

While neither the PS propagator  $K(q, p, t | q_0, p_0, t_0)$  nor the position space propagator  $K(q, t | q_0, t_0)$  can be analytically evaluated in general for Lagrangians with arbitrary time-dependence, methods can be developed for TD systems satisfying certain suitable conditions, e.g. systems possessing invariants.

We consider a TD system characterized by a Hamiltonian of the form  $H(q, p, t) = p^2/2m + V(q, t)$  and the objective is to find the solution of the resulting equation for the PS distribution given by eq. (8). Now, assuming the potential  $V(q, t)$  to be such that there exists an invariant  $I(q, p, t)$  for this TD problem, the corresponding Wigner operator,  $\hat{I}_w$  defined through eq. (5) clearly satisfies the operator equation of motion of the form of eq. (12), viz.

$$(d/dt)\hat{I}_w = (\partial/\partial t)\hat{I}_w - (i\hbar)^{-1}[\hat{H}_w\hat{I}_w - \hat{I}_w\hat{H}_w] = 0. \quad (15)$$

The PS propagator  $K(q, p, t | q_0, p_0, t_0)$  for this system can be obtained as an extension in terms of the PS eigenstates of the invariant operator [5], given by

$$(1/\hbar)(\hat{I}_w - \hat{I}_w^*)f_{nm}(q, p, t) = a_{nm}f_{nm}(q, p, t). \quad (16)$$

For stationary states, the PS eigenfunctions  $f_{nm}$  can be defined through an off-diagonal generalization of eq. (1), viz.

$$f_{nm} = (2\pi\hbar)^{-1} \int dy \exp[ip y/\hbar] \langle q - y/2 | \hat{\rho}_{nm} | q + y/2 \rangle, \quad (17)$$

where  $\hat{\rho}_{nm} = |n\rangle\langle m|$  represents the density matrix operator characterizing the  $n$ -th and  $m$ -th eigenstates of the eigenvalue problem in the Hilbert space of the wavefunction, i.e.  $\hat{I}\psi_n = a_n\psi_n$ . The eigenvalues  $\{a_{nm}\}$  are related [5,10] to the QM eigenvalues  $\{a_n\}$  by  $a_{nm} = (1/\hbar)(a_n - a_m)$ .

In our earlier work [5], we have employed the operator eq. (15) and the Hermitian nature of the operator  $(\hat{I}_w - \hat{I}_w^*)$  to prove that the eigenvalues  $\{a_{nm}\}$  (which are obviously real) have no explicit time-dependence. Using this result and the fact that the PS eigenfunctions  $\{f_{nm}\}$  form an orthonormal complete set, satisfying  $(2\pi\hbar)^{-1} \int dq \int dp f_{nm} f_{n'm'}^* = \delta_{nm'} \delta_{mm'}$ , one obtains after some algebra the general PS eigenfunction expansion for the propagator.

As an illustration, let us consider TD systems possessing an invariant quadratic in the momentum  $p$  which corresponds to a general TD potential of the form [11]

$$V(q, t) = [(\ddot{\alpha}\beta/\alpha) - \ddot{\beta}]q - (\ddot{\alpha}/2\alpha)q^2 + \alpha^{-2}\gamma((q - \beta)/\alpha), \quad (18)$$

where  $\alpha(t)$ ,  $\beta(t)$  and  $\gamma((q - \beta)/\alpha)$  are arbitrary functions of their respective arguments. The invariant associated with this system is of the form [11]

$$I(q, p, t) = (1/2) [\alpha(p - \dot{\beta}) - \dot{\alpha}(q - \beta)]^2 + \gamma((q - \beta)/\alpha). \quad (19)$$

Following Dhara and Lawande [6], one can easily obtain the PS propagator  $K(q, p, t | q_0, p_0, t_0)$  as the Wigner transform

$$\begin{aligned} K(q, p, t | q_0, p_0, t_0) &= K_0(\zeta, \pi, \tau | \zeta_0, \pi_0, \tau_0) \\ &= \iint d\eta d\eta_0 \exp[(i\pi\eta/\hbar) - (i\pi_0\eta_0/\hbar)] K_0^*(\zeta + \eta/2, \tau | \zeta_0 + \eta_0/2, \tau_0) \\ &\quad K_0(\zeta - \eta/2, \tau | \zeta_0 - \eta_0/2, \tau_0), \end{aligned} \quad (20)$$

where in the RHS, there appear the new coordinate, momentum and time variables defined as

$$\zeta = [q - \beta(t)]/\alpha(t) \quad (21)$$

$$\pi = \alpha(t)[p - \dot{\beta}(t)] - \dot{\alpha}(t)[q - \beta(t)] \quad (22)$$

$$\tau = \int^t dt' \alpha^{-2}(t'), \quad (23)$$

and  $K_0(\zeta, \pi, \tau | \zeta_0, \pi_0, \tau_0)$  and  $K_0(\zeta, \tau | \zeta_0, \tau_0)$  are respectively the PS propagator and the coordinate space propagator corresponding to a modified simpler time independent Lagrangian [6]  $L_0$  in the new space time variables given by

$$L_0 = (1/2)(d\zeta/d\tau)^2 - \gamma(\zeta). \quad (24)$$

It is clear that the momentum  $p_\zeta$ , defined through  $L_0$  in eq. (24) is canonical to the coordinate  $\zeta$  and is given by

$$p_\zeta = (d\zeta/d\tau) = \alpha[p - \dot{\beta}] - \dot{\alpha}[q - \beta], \quad (25)$$

and hence the Hamiltonian

$$H_s^0(\zeta, p_\zeta, \tau) = (1/2)p_\zeta^2 + \gamma(\zeta) \quad (26)$$

is identical to the invariant  $I(\zeta, p_\zeta, \tau)$  (see eq. (19)).

The propagator  $K_0(\zeta, \pi, \tau | \zeta_0, \pi_0, \tau_0)$  and hence the propagator  $K(q, p, t | q_0, p_0, t_0)$  can be expanded in terms of the PS eigenfunctions  $f_{nm}(\zeta, \pi)$  of the invariant operator (equivalent to the Hamiltonian in  $(\zeta, p_\zeta)$  space) as

$$K_0(\zeta, \pi, \tau | \zeta_0, \pi_0, \tau_0) = \sum_n \sum_m \exp[(i/\hbar)a_{nm}(\tau - \tau_0)] f_{nm}^*(\zeta_0, \pi_0) f_{nm}(\zeta, \pi), \quad (27)$$

where  $f_{nm}(\zeta, \pi)$  and  $a_{nm}$  are the PS eigenfunctions and the eigenvalues defined by an equation similar to eq. (16), with  $f_{nm}$  depending on  $(\zeta, \pi)$  coordinates and  $\hat{I}_w$  being the Wigner operator corresponding to the invariant of eq. (19).

For Hamiltonians characterized by potentials of the form of eq. (18), *i.e.* with TD invariants of the form of eq. (19), one can thus evaluate the propagator using eqs. (27) and (20) and hence the PS function from eq. (13).

The most interesting example of a TD system possessing invariants quadratic in momentum is that of a time-dependent harmonic oscillator with a TD frequency  $\omega(t)$ , described by the Hamiltonian

$$H = p^2/2 + (1/2)\omega^2(t)q^2. \quad (28)$$

The TD invariant  $I(t)$  associated with this system is given by

$$I(q, p, t) = (1/2)[(\alpha p - \dot{\alpha} q)^2 + k(q/\alpha)^2], \quad (29)$$

where  $k$  is a constant and  $\alpha(t)$  satisfies

$$\ddot{\alpha} + \alpha\omega^2(t) = k/\alpha^3. \quad (30)$$

The invariant operator (29) can also be expressed in the simple form

$$I = (1/2) [P^2 + kQ^2] \quad (31)$$

in terms of the new variables  $Q$  and  $P$  obtained through the canonical transformations

$$Q = q/\alpha; \quad P = \alpha p - \dot{\alpha} q \quad (32)$$

Eq. (31) suggests that the invariant in the transformed variables plays the role of Hamiltonian for a time-independent harmonic oscillator.

Interestingly, the propagator for the time-dependent or time-independent harmonic oscillator can also be derived from that of a free particle. Choosing  $\beta = \gamma = 0$

and  $(\ddot{\alpha}/\alpha) = -\omega^2(t)$ , one has  $V(q, t) = (1/2) \omega^2(t)q^2$  from eq. (18) and  $I(q, p, t) = (1/2) [\alpha p - \dot{\alpha}q]^2$  from eq. (19). The phase space propagator  $K(q, p, t | q_0, p_0, t_0)$  can then be calculated using eq. (20), the propagator  $K_0(\zeta, \tau | \zeta_0, \tau_0)$  now denoting the free particle propagator in  $(\zeta, \tau)$  space corresponding to the Lagrangian  $L_0 = (1/2)(d\zeta/d\tau)^2$  (see eq. (24)). Using the standard expression of the position space propagator  $K_0$  given by

$$K_0(\zeta, \tau | \zeta_0, \tau_0) = [2\pi i\hbar(\tau - \tau_0)]^{-1/2} \exp\left[(i/2\hbar)(\zeta - \zeta_0)^2/(\tau - \tau_0)\right], \quad (33)$$

one thus obtains the PS propagator

$$K_0(\zeta, \pi, \tau | \zeta_0, \pi_0, \tau_0) = [2\pi\hbar/(\tau - \tau_0)] \delta(\pi - (\zeta - \zeta_0)/(\tau - \tau_0)) \delta(\pi_0 - (\zeta - \zeta_0)/(\tau - \tau_0)), \quad (34)$$

which can be rewritten in terms of the original variables as

$$K(q, p, t | q_0, p_0, t_0) = 2\pi\hbar [(\tau - \tau_0) |\alpha(t)| |\alpha(t_0)|]^{-1} \delta\left(p - \frac{\dot{\alpha}(t)}{\alpha(t)} q - [\alpha(t_0)q - \alpha(t)q_0] / [\alpha(t_0)\alpha^2(t)(\tau - \tau_0)]\right) \delta\left(p_0 - \frac{\dot{\alpha}(t_0)}{\alpha(t_0)} q_0 - [\alpha(t_0)q - \alpha(t)q_0] / [\alpha^2(t_0)\alpha(t)(\tau - \tau_0)]\right). \quad (35)$$

The quantity  $\alpha(t)$  and  $\tau(t)$  can be obtained from solution of the differential eq. (30) and from eq. (23) respectively. The PS distribution function  $f(q, p, t)$  can thus be calculated using eqs. (13) and (35) together with the initial condition  $f(q_0, p_0, t_0)$ .

As a general case, one can consider  $\omega(t) = \text{constant}$ , corresponding to a time-independent harmonic oscillator. For this case,  $\ddot{\alpha} + \omega^2\alpha = 0$  (eq. (30) with  $k = 0$ ) has a particular solution  $\alpha(t) = \sin \omega t$  and eq. (23) leads to the result  $\tau(t) = -(\cot \omega t)/\omega$ . Eq. (35) then yields

$$K_{\text{HO}}(q, p, t | q_0, p_0, t_0) = [2\pi\hbar\omega / \sin \omega(t - t_0)] \delta(p - \omega[q \cos \omega(t - t_0) - q_0] / \sin \omega(t - t_0)) \delta(p_0 - \omega[q - q_0 \cos \omega(t - t_0)] / \sin \omega(t - t_0)), \quad (36)$$

which is the PS propagator for a time-independent harmonic oscillator, obtained here in a simple manner through a free particle propagator.

The propagator can also be evaluated in terms of the contribution of the classical path to it. We rewrite the quantum Liouville eq. (8) by separating out the classical operator on the LHS, i.e.

$$\hat{L}_0 f(q, p, t) \equiv [(\partial/\partial t) + (p/m)(\partial/\partial q) - (\partial V/\partial q)(\partial/\partial p)] f(q, p, t) = \theta(q, p, t) \quad (37)$$

where the inhomogeneous term  $\theta$  on the RHS is given by

$$\theta(q, p, t) \equiv \left[ (i\hbar)^{-1} \{ V(q - (\hbar/2i)(\partial/\partial p)) - V(q + (\hbar/2i)(\partial/\partial p)) \} \right. \\ \left. - (\partial V/\partial q)(\partial/\partial p)f(q, p, t) \right]. \quad (38)$$

In absence of this term, eq. (37) represents the classical Liouville equation. The classical limit of the PS propagator  $K_{c1}(q, p, t | q_0, p_0, t_0)$  is essentially the causal Green's function of the adjoint classical operator  $\hat{L}_0^+$ .

Therefore, one can write

$$f(q, p, t) = \iint dq' dp' K_{c1}(q, p, t | q', p', t') f(q', p', t') \\ + \int dt' \iint dq' dp' K_{c1}(q, p, t | q', p', t') \theta(q', p', t'), \quad (39)$$

where the first term is analogous to eq. (13). Now, since  $f(q, p, \hbar)$  is defined by the transformation of eq. (1), one can reexpress  $\theta$  of eq. (38) in terms of an integral involving  $f(q, p, \hbar)$  instead of the derivatives. Thus, one has

$$\theta(q, p, t) = (2\pi\hbar)^{-1} \int dy \left[ (1/i\hbar) \{ V(q - y/2) - V(q + y/2) + y(\partial V/\partial q) \} \right. \\ \left. \exp[i p y / \hbar] \langle q - y/2 | \hat{p} | q + y/2 \rangle \right] \quad (40a)$$

$$= (2\pi i \hbar^2)^{-1} \int dy \int dp' \left[ \{ V(q - y/2) - V(q + y/2) + y(\partial V/\partial q) \} \right. \\ \left. \exp[i(p - p')y/\hbar] f(q, p', t), \right] \quad (40b)$$

where the second equality has been obtained by using the inverse transform of eq. (1). Substituting eq. (40) in eq. (39), we obtain

$$f(q, p, t) = \int dq' dp' K_{c1}(q, p, t | q', p', t_0) f(q', p', t_0) \\ + (2\pi i \hbar^2)^{-1} \int dt' \int dq' \int dp' K_{c1}(q, p, t | q', p', t') \\ \left[ \int dy \int dp'' \{ V(q' - y/2) - V(q' + y/2) + y(\partial V/\partial q') \} \right. \\ \left. \exp[i(p' - p'')y/\hbar] f(q', p'', t'), \right] \quad (41)$$

which is an integral equation for  $f(q, p, \hbar)$  in terms of the propagator  $K_{c1}$  of the classical adjoint Liouville equation. The first term on the RHS gives the solution of the classical Liouville equation while the next term gives the quantum contribution. By iterative expansion, one obtains the quantum corrections of increasing orders in  $\hbar$  of the form

$$f(q, p, t) = f_{c1}(q, p, t) \sum \hbar^n f_n^q(q, p, t | q', p', t_0), \quad (42)$$



where  $f_n^q$  represents the quantum correction factors, with  $f_0^q = 1$ .

## 5. Concluding remarks

The phase space formalism provides a classical-like conceptual framework for discussing quantum phenomena and is a useful tool not only for the study of interpretive aspects [12], but also for calculations. Here, the quantum corrections are explicit, thus providing insight into various approximation schemes for solving the quantum equations of motion. This might enable one to employ some of the methods of approximation or expansion used in classical cases to the problems involving quantum effects [13].

The importance of the Heisenberg-like operator equation of motion [5] in phase space introduced earlier is further illustrated here through its use in obtaining newer methods of direct solution for the PS distribution function. A direct solution is important for the PS formalism to be an independent representation in its own right.

The example discussed here is only illustrative and the form of eq. (18) may not be as restrictive as it first appears to be, since more general cases can often be reduced [14] to this quadratic form through canonical transformations. Moreover, the special case of time-dependent harmonic oscillator itself finds important applications in a number of physical problems. For example, the dynamical variables associated with the motion of a charged particle under the action of a uniform magnetic field of arbitrary time-dependence, the associated induced electric field and also an electric field due to an arbitrary time-dependent uniform charge distribution, are simply related to those of the time-dependent harmonic oscillator through a simple transformation [15].

While the present work deals with a single particle in one dimension, its generalization to higher dimensions is straightforward. For many-particle systems, however, due to the presence of interparticle interaction terms, the distribution function has to be obtained either through Hartree-Fock like approximate single-particle schemes or by developing a formally exact single-particle density functional framework [16] in phase space [17].

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